# **Prediction of AMOS Observations of Shuttle Engine Firing**

Matthew Braunstein Lawrence Bernstein

Spectral Sciences, Inc. 4 Fourth Avenue Burlington, MA 01803

Scientific Report No. 5

8 November 2005

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.



AIR FORCE RESEARCH LABORATORY Space Vehicles Directorate 29 Randolph Road AIR FORCE MATERIEL COMMAND Hanscom AFB, MA 01731-3010 This technical report has been reviewed and is approved for publication.

AFRL-VS-HA-TR-2005-1184

/signed/

/signed/

RAINER DRESSLER
Contract Manager

JOEL B. MOZER, Chief Space Weather Center of Excellence

This report has been reviewed by the ESC Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS).

Qualified requestors may obtain additional copies from the Defense Technical Information Center (DTIC). All others should apply to the National Technical Information Service.

If your address has changed, if you wish to be removed from the mailing list, or if the addressee is no longer employed by your organization, please notify AFRL/VSIM, 29 Randolph Rd., Hanscom AFB, MA 01731-3010. This will assist us in maintaining a current mailing list.

Do not return copies of this report unless contractual obligations or notices on a specific document require that it be returned.

Using Government drawings, specifications, or other data included in this document for any purpose other than Government procurement does not in any way obligate the U.S. Government. The fact that the Government formulated or supplied the drawings, specifications, or other data does not license the holder or any other person or corporation; or convey any rights or permission to manufacture, use, or sell any patented invention that may relate to them.

## REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
08-11-2005	Scientific Report No. 5	11/10/05 - 11/10/05
4. TITLE AND SUBTITLE		5a. CONTRACT NUMBER
		F19628-00-C-0006
Prediction of AMOS Observati	ions of Space Shuttle Engine Firing	5b. GRANT NUMBER
		5c. PROGRAM ELEMENT NUMBER
		SC. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	*	5d. PROJECT NUMBER
		1010
Matthew Braunstein and Lawr	rence Bernstein	5e. TASK NUMBER
		RS
		5f. WORK UNIT NUMBER
		Al
7. PERFORMING ORGANIZATION NAM	IE(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT NUMBER
Spectral Sciences, Inc.		Homber
4 Fourth Avenue		
Burlington, MA 01803-3304		SSI-SR-270
burnington, with 0 1000 0004		GGI GIV 270
9. SPONSORING / MONITORING AGEN	ICY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
Air Force Research Laboratory		AFRL/VSBXT
29 Randolph Road		No.   No.
Hanscom AFB, MA 01731-3010		11. SPONSOR/MONITOR'S REPORT
		NUMBER(S)
		NUMBER(S) AFRL-VS-HA-TR-2005-1184

Approved for public release; distribution unlimited.

#### 13. SUPPLEMENTARY NOTES

In this report, we discuss predictions for observations of on-orbit Shuttle plumes from the Air Force Maui Optical Station (AMOS). The focus is a 2-5 µm spectral region. The major light-producing mechanisms considered are O+H2O -> 20H\* and O+H2O -> H2O\*+O. Recently computed velocity-dependent cross sections for these mechanisms are used in conjunction with the Spacecraft Orbiter Contamination Representation Accounting for Transiently Emitted Species (SOCRATES) flow-field code to predict the emissions for a PRCS (Primary Reaction Control System) engine for various angles of attack and velocities. The impact of atmospheric attenuation is discussed. Signal-to-noise estimates are presented for candidate spectral sensors installed at AMOS.

15. SUBJECT TERMS Plume, Emission		le, AMOS, Sensor	, SOCRATES		,
16. SECURITY CLASS	SIFICATION OF:		17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON R. Dressler
a. REPORT UNCLASSIFIED	b. ABSTRACT UNCLASSIFIED	c. THIS PAGE UNCLASSIFIED	SAR	22	19b. TELEPHONE NUMBER (include area code) (781) 377-2332

# **CONTENTS**

1.	Introduction	1
2.	Observation Scenario	2
3.	Chemical Mechanisms	3
4.	Total Source (Un-Attenuated) Signal	6
5.	Atmospheric Attenuation and Spectral Signals	7
6.	Instrumentation	0
	Conclusions and Future Work	
8.	References	4

# **FIGURES**

1.	Shuttle Engine Firing Observation Scenario
2.	Energy Level Diagram of Low-Lying Triplets (solid lines) and Singlets (dashed lines) Showing Reagents, Transition States, and Products for O + H <sub>2</sub> O Collisions
3.	Cross Sections for the Reaction, $O + H_2O \rightarrow OH(v) + OH(v)$ , as a Function of Collision Velocity
4.	Cross Sections for the Reaction, $O + H_2O \rightarrow O + H_2O^*$ , as a Function of Collision Velocity
5.	Photon Production Efficiency per Collision and Total Source Signal in Photons s <sup>-1</sup> as a Function of Velocity for PRCS Engine Firings
6.	Normalized Spectral Radiance from OH(v) (black curve) and H <sub>2</sub> O* (blue curve) at 8 km s <sup>-1</sup> Relative Collision Velocity
7.	Source OH(v) + H <sub>2</sub> O* Relative Spectral Radiance at 8 km s <sup>-1</sup> Relative Collision Velocity 8
8.	Normalized Spectral Radiance from OH(v) (black curve) and H <sub>2</sub> O* (blue curve) at 11 km s <sup>-1</sup> Relative Collision Velocity
9.	Source OH(v) + H2O* Relative Spectral Radiance at 11 km s-1 Relative Collision Velocity
10.	Estimated Signal-to-Noise for Various Spectrometer Spectral Resolutions and Measurement Times
	TABLES
1.	Total Signal Estimates for Shuttle PRCS Engine Firings Including Atmospheric  Attenuation in the 2-5 µm pass-band
2.	ABB 254 FTIR Spectrometer Specifications

# **ACKNOWLEDGEMENTS**

We acknowledge support through a Small Business Innovative Research (SBIR) award from the Missile Defense Agency (MDA) Contract No. F04611-03-C-0015 and support from Air Force Research Laboratory (AFRL) through contract F19628-00-C-0006. We also acknowledge key technical contributions from M. Venner (AFRL) and R. Dressler (AFRL).

#### 1. INTRODUCTION

Engine firings of the Space Shuttle Primary Control System (PRCS) thrusters can give rise to radiation observable from ground-based telescopes such as the Air Force Maui Optical Station (AMOS). Such observations would yield valuable information on the environment near the spacecraft during engine operation. The radiation and the mechanisms that produce it are also important to characterize because such radiation can be a significant background noise source for telescopes mounted on spacecraft in low-Earth-orbit or LEO in general [1]. Furthermore, observations of radiation associated with engine firings can give valuable information on fundamental chemical reactions that can be studied over the very large length scales, high energies, and rarefied conditions that are achievable in space but are especially difficult to reproduce in ground-based laboratories.

Radiation associated with Space Shuttle engine firings extending from the ultraviolet region through the infrared has been observed from ground-based, satellite, and on-board sensors [2-9]. The mechanisms that give rise to this radiation are quite diverse. They include combustion products of the Space Shuttle engine reacting (either through collisional excitation or chemical reaction) with atomic oxygen in the atmosphere to produce excited state species that then radiate, absorption of sunlight by combustion products that become excited and then radiate, reflection of sunlight from un-combusted engine fuel droplets, and several others. The observed signals appear to be a sensitive function of altitude and atmospheric conditions, spacecraft relative velocity with the atmosphere, and spectral wavelength region. The spatial scale of these signals can extend over several kilometers, reflecting the collision mean-free-path associated with engine exhaust constituents colliding with the atoms and molecules in the rarefied LEO atmosphere.

In this work, we focus on radiation observable in the  $2-5\mu m$  (short-wave infrared) region. In this region there are two basic mechanisms known to give rise to observable signals. They are chemical reaction of  $H_2O$  from the Shuttle exhaust and atmospheric atomic oxygen to produce excited OH which then radiates,

$$O(^{3}P) + H_{2}O(X,^{1}A_{1}) \rightarrow OH(X,^{2}\Pi) + OH(X,^{2}\Pi), \Delta H = +16.9 \text{ kcal mol}^{-1},$$
 (1)

and collisions of H<sub>2</sub>O from the Shuttle exhaust with atmospheric atomic oxygen to produce internally excited H<sub>2</sub>O (collisional excitation) which then radiates,

$$O(3P) + H2O(X,1A1, (v1v2v3,JK)) \rightarrow O(3P) + H2O(X,1A1(v1'v2'v3',J'K')).$$
 (2)

Bernstein *et al.* [6] have shown, through analysis of space experiments and laboratory data, that the observed radiation from  $O(^3P) + H_2O(X,^1A_1)$  collisions may be consistent with either (1) or (2) depending on the collision velocity. Other studies have attributed all such radiation to Reaction (2). It is particularly difficult to distinguish between (1) and (2) in the 2-5  $\mu$ m spectral region because  $OH(X,^2\Pi)$  and  $H_2O(X,^1A_1)$  have highly overlapping spectral distributions there.

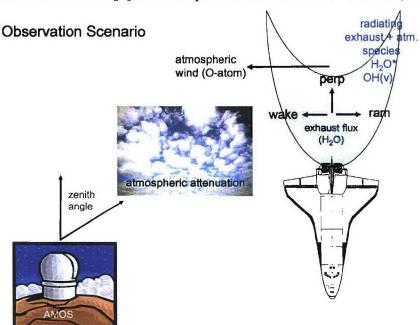
The present work leverages recently published work [10] on the detailed chemistry of O + H<sub>2</sub>O to provide signal estimates of PRCS engine firings that could be observed from AMOS. We take into account significant atmospheric absorption effects, and show predicted source and apparent spectra and an upper bound on the total observed signal. These calculations are then used to establish sensitivity requirements and assess measurement feasibility with available instrumentation. It is expected that the results will be of great value in preparing for future

AMOS observations of Space Shuttle firings. In Section 2, we discuss observation scenarios. In section 3, we review detailed data on the chemical mechanisms that give rise to the radiation in order to develop an estimate of the total source signal that is discussed in section 4. In section 5, we discuss atmospheric effects and their impact on the detailed observable spectra and give an estimate of the total apparent signal. In section 6, we discuss instrumentation and signal to noise considerations. In Section 7, we give conclusions and discuss possible future work.

#### 2. OBSERVATION SCENARIO

The observation scenario is shown in Figure 1. Although the exact conditions will depend on the time and details of the particular mission, bracketing general conditions based on previous similar events will be examined. The results from such an analysis can easily be extended to include a particular observation scenario. Many of these observation parameters are derived from an analysis associated with the STS-63 mission where on-board telescopes were used to examine UV radiation associated with Shuttle exhaust [9]. At an operational altitude of ~390 km, the

atmosphere is dominated by oxygen atoms whose density is ~5 e13 m<sup>-3</sup> and whose temperature varies 700-1000K. between Assuming co-rotation of thermosphere, the spacecraft velocity with respect to the atmosphere ranges between 7.37 and  $7.38 \times 10^3$  m s<sup>-1</sup> for a West-East orbit, depending on the orbiter latitude. We focus on engine firings from the PRCS engines, which use N<sub>2</sub>O<sub>4</sub> oxidizer monomethyland hydrazine [(MMH, chemical formula (CH<sub>3</sub>)HN-NH<sub>2</sub>)] fuel and have an 870 lbf thrust. The combustion gaseous products emanating from the nozzle exit include



**Figure 1.** Shuttle engine firing observation scenario. Engine exhaust, consisting mostly of  $H_2O$ , interacts with O-atom in the atmosphere to produce internally excited species, OH(v) and  $H_2O^*$ . The radiative decay of these excited species is attenuated by the atmosphere and observed from AMOS in the 2-5  $\mu$ m region.

 $H_2O$ , CO,  $H_2$ , and  $N_2$ , with  $H_2O$  at about 1/3 the total mole fraction. The total flux of exhaust gaseous species is ~4.26e25 sec<sup>-1</sup>. An axial exhaust velocity of  $3.5 \times 10^3$  m s<sup>-1</sup> is assumed, which originates from the exit velocity of  $3 \times 10^3$  m s<sup>-1</sup> plus an additional  $0.5 \times 10^3$  m s<sup>-1</sup> attained in the vacuum expansion. The relative speed between the oxygen atoms in the atmosphere and the exhausting  $H_2O$ , which determines the available energy of the collision, is key in determining the level of signal observed. The relative speed is a vector sum of the atmospheric O-atom and  $H_2O$  exhaust velocities. It can vary greatly depending on whether the PRCS engines are firing along the wind direction (0 degree or "wake" firing), perpendicular to the wind direction (90 degree or

"perpendicular" firing) or against the atmospheric wind direction (180 degree or "ram" firing). For the conditions given above, the relative O-atom/H<sub>2</sub>O collision speed is 3.9 km s<sup>-1</sup>, 8.2 km s<sup>-1</sup> and 10.9 km s<sup>-1</sup> for wake, perpendicular, and ram firings, respectively. We also note that the atmospheric temperature implies a spread of O-atom speeds of approximately 1 km s<sup>-1</sup>, so that the relative collision speeds will have a ~1.0 km s<sup>-1</sup> spread around the center values given above. We also note that attenuation effects due to absorption of radiation by CO<sub>2</sub> and H<sub>2</sub>O in the atmosphere will be appreciable, and these effects must be taken into account in such an observation scenario.

#### 3. CHEMICAL MECHANISMS

To illustrate the chemical mechanisms involved which produce the observable radiation, Figure 2 shows an energy level diagram for  $O + H_2O$  collisions with reagents on the left and products on the right against a velocity and energy scale. Creation of product OH(v) and  $H_2O^*$  requires significant translational energy. The reagent  $H_2O$  has negligible internal energy after expanding into the rarefied atmosphere and the OH(v) and  $H_2O^*$  are higher in energy than the cold reagents by a large amount. This implies that wake engine firings, which have a relative  $OH_2O$  collision speed of 3.9 km s<sup>-1</sup>, will have extremely small signals, as this energy is not enough to produce OH(v>0) and is just above threshold for  $H_2O^*$ . Radiation in the 2-5  $\mu$ m band of interest will occur for creation of populations of OH(v>0) (vibrational excitation beyond the ground state) and for creation of vibrationally excited  $H_2O$ , which we denote here as  $H_2O^*$ .  $H_2O$  has three vibrational modes  $(v_1, v_2, v_3)$ . Excitation into  $v_1$  and  $v_3$  (~10.5 kcal mol<sup>-1</sup> energy) will fall into the band of interest, while excitation into  $v_2$ , which has a lower energy, will be centered near 6.3  $\mu$ m (4.5 kcal mol<sup>-1</sup>).

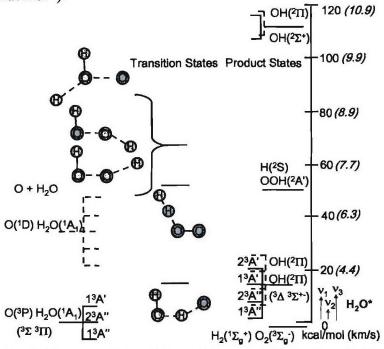


Figure 2. Energy level diagram of low-lying triplets (solid lines) and singlets (dashed lines) showing reagents, transition states, and products for  $O + H_2O$  collisions [10]. The energy and corresponding relative collision velocities are shown in parentheses with respect to the  $O(^3P) + H_2O(X,^1A_1)$  asymptote at zero energy. The energies of the fundamental vibrational modes of  $H_2O$  are also shown.

To estimate the observed signal, we adopt a simple model for the total radiation output under steady-state (long engine firings) and single-collision (very high altitude) conditions. The spatial region of the radiation will extend several kilometers, and it will be very non uniform. We do not address the spatial variation of the signal here, and we assume that we are capturing all the available radiation. As outlined in [6] and [10], space-based measurements are characterized by a steady-state out-gassing or exhausting source of  $H_2O$  with a known or assumed rate,  $N_{H_2O}$  (number of  $H_2O$  per second), interacting with atomic oxygen in the atmosphere. The signal is observed through a somewhat opaque atmosphere integrated over a wavelength band and characterized by a transmittance,  $T_{A\lambda}$ . The observed steady-state intensity,  $I_{A\lambda}^{space}$  (photons s<sup>-1</sup>), can be written,

$$I_{\Delta\lambda}^{space} \approx \left[\frac{\sigma^*}{\sigma_{tot}}\right] N_{H_2O} T_{\Delta\lambda} \,,$$
 (3)

where  $\sigma_{tot}$  is the total (reactive and non-reactive) collision cross section for O + H<sub>2</sub>O and  $\sigma^*$  is the photon excitation cross section which includes all contributions due to photon cascades from multi-quantum excited states. Equation 3 assumes all H<sub>2</sub>O molecules collide with atmospheric atomic oxygen once, and that all radiation from these collisions (after being attenuated by the

atmosphere) is detected. The ratio,  $\left[\frac{\sigma^*}{\sigma_{tot}}\right]$ , is the efficiency of producing a photon for a single

collision of  $O + H_2O$ . For detection in the 2-5  $\mu m$  spectral region, the intensity will be sensitive to single vibrational quantum changes, so we write the efficiency as,

$$\left[\frac{\sigma^*}{\sigma_{tot}}\right] = \frac{1}{\sigma_{tot}} \sum_{species} \sum_{v=1}^{species} v \sigma_v^{species} , \qquad (4)$$

where v is the vibrational quantum number,  $\sigma_v^{species}$  is the cross section to a particular vibrational state of either collisionally excited  $H_2O$  or reaction product OH radiating in the detection band. It is important to emphasize that observations will include contributions from both species. The second sum extends over all possible excited vibrational levels of a given species. Space-based measurements usually assume or otherwise employ models to estimate values for  $N_{H_2O}$ ,  $T_{\Delta\lambda}$  and  $\sigma_{tot}$ , and from the observed intensity,  $I_{\Delta\lambda}^{space}$ , report a photon excitation cross section,  $\sigma^*$ . Therefore, uncertainties in the estimated values of  $N_{H_2O}$ ,  $T_{\Delta\lambda}$  and  $\sigma_{tot}$  are reflected in reported  $\sigma^*$ .

The key factor in determining signal levels is the efficiency (Eq. 4). To estimate this efficiency, we use the recently determined  $O + H_2O \rightarrow OH(v) + OH(v)$  cross sections (Eq. 1), obtained in [10]. These were obtained from computational chemistry modeling of the potential energy surfaces of  $O + H_2O$  followed by classical trajectory dynamics calculations to determine cross sections. The results of this modeling showed good agreement with available data, although such data is quite sparse. Figure 3 shows the cross section as a function of collision velocity derived from the cross sections reported in [10]. It rises steeply from an energy threshold near 4 km s<sup>-1</sup> for the OH(v=0) product. As the energy increases above the thresholds for the higher OH(v) states, the higher OH states begin to contribute. Also shown is the  $O + H_2O$  total cross section,  $\sigma_{tot}$ , taken from [6],  $\sigma_{tot} = 2.7e - 15\sqrt{2./v_r}$ , where  $v_r$  is the relative collision speed in units of km s<sup>-1</sup>, and the resulting total cross section is in units of cm<sup>2</sup>. These values for the  $O + H_2O$  total cross section are very close to those derived in the analysis of observations involving the Russian space station Mir [11].

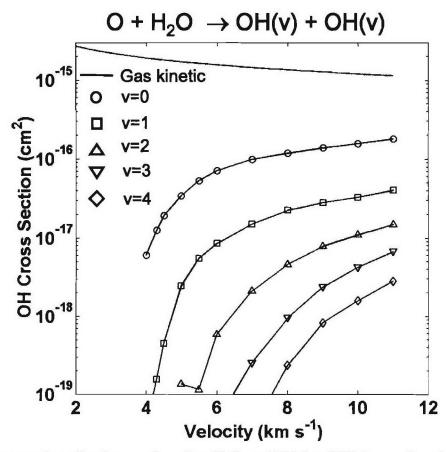


Figure 3. Cross sections for the reaction,  $O + H_2O \rightarrow OH(v) + OH(v)$ , as a function of collision velocity, derived from [10]. The  $H_2O$  is considered internally cold after undergoing a vacuum expansion. Also shown is the gas kinetic (total) cross section for  $O + H_2O$  collisions from [6].

Figure 4 shows the cross sections for excitation of  $H_2O$ ,  $O + H_2O \rightarrow O + H_2O^*$  (Eq. 2). These results are new and use the classical trajectory methods outlined in [10] on the same potential surface. The classical trajectory methods used in [10], although convenient for many applications, are not easily amenable to finding vibrationally resolved cross sections for polyatomic molecules, such as H<sub>2</sub>O. We, therefore, use an ('ad-hoc') method of estimating the H<sub>2</sub>O\* efficiency from the classical trajectory data. Excitation cross sections are obtained by summing all trajectories where the product H<sub>2</sub>O\* has more vibrational energy than the groundstate vibrational bin (27.07 kcal mol<sup>-1</sup>). The curve labeled v'=1 corresponds to H<sub>2</sub>O\* whose vibrational energy lies between 27.07 and 31.92 kcal mol<sup>-1</sup>. The higher bins are incremented in steps of the same width, 4.85 kcal mol<sup>-1</sup>, the approximate width of the 6.3 µm bin. All bins are labeled as v'=n, where n=1 is the first bin above the vibrational excitation threshold. These excitation cross sections are actually distributed among all the H<sub>2</sub>O vibrational excited states  $(v_1,v_2,v_3)$ . We partition the total  $H_2O^*$  ( $H_2O$  v>0) cross section into that contributing to 2-5 µm radiation (H<sub>2</sub>O 2.7 µm) and that falling outside (dominated by 6.3 µm) in the amounts of 0.15 and 0.85, respectively. This assumption is based on a 'best guess' and represents the weakest part of the signal estimate. We note that near threshold, at least, the relative amounts of 6.3 µm and 2.7 µm H<sub>2</sub>O will not be constant as assumed here.

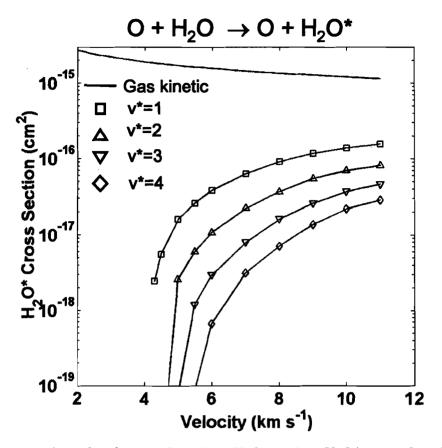


Figure 4. Cross sections for the reaction,  $O + H_2O \rightarrow O + H_2O^*$ , as a function of collision velocity, derived using the methods of [10]. The product  $H_2O^*$  is split into excited vibrational bins, as discussed in the text. Also shown is the gas kinetic (total) cross section for  $O + H_2O$  collisions from [6].

### 4. TOTAL SOURCE (UN-ATTENUATED) SIGNAL

The data shown in Figures 3 and 4 were translated into total photon efficiencies (Eq. 4), and total signal in units of photon  $s^{-1}$  (Eq. 3) at the source (excluding the  $T_{\Delta\lambda}$  transmission factor) assuming the PRCS engine parameters previously discussed. These results are shown in Figure 5 as a function of collision velocity. There are three curves. The curves labeled  $H_2O$  2.7  $\mu m$  and OH 2.8  $\mu m$  contribute to the 2-5  $\mu m$  pass-band. They start from a relatively small value near threshold and increase rapidly with collision velocity. It is remarkable that the  $H_2O$  2.7  $\mu m$  contribution and the OH 2.8  $\mu m$  contribution are nearly identical above threshold. This means that in the total source signal, they will contribute about equally. The range of wake, perpendicular, and ram velocities are also shown in this figure. It is clear that wake firings will have a very weak signal, however the source signal will increase greatly as the engine fires into the atmospheric wind (ram direction). This behavior mirrors the threshold effects evident in the vibrational excitation cross sections shown in Figures 3 and 4.

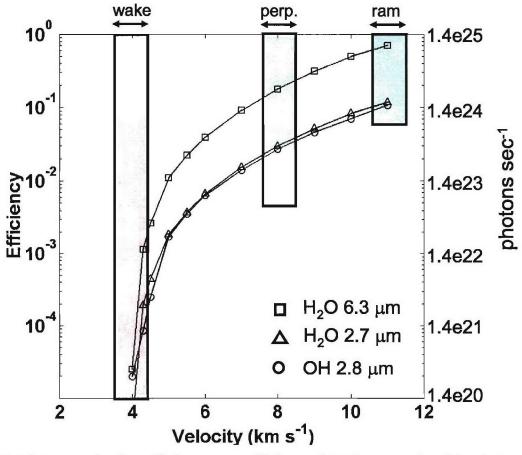


Figure 5. Photon production efficiency per collision and total source signal in photons s<sup>-1</sup> as a function of velocity for PRCS engine firings. The  $H_2O^*$  contribution has been split into  $H_2O$  2.7  $\mu m$  and  $H_2O$  6.3  $\mu m$  contributions. The OH(v) contribution here is called 'OH 2.8  $\mu m$ '. The OH 2.8  $\mu m$  and  $H_2O$  2.7  $\mu m$  curves contribute to the 2-5  $\mu m$  pass-band.

# 5. ATMOSPHERIC ATTENUATION AND SPECTRAL SIGNALS

Figure 6 shows spectra computed for OH(v) and  $H_2O^*$  which have been separately normalized to 1.0, as well as the atmospheric transmittance from a MODTRAN [12] calculation at a 60 degree zenith angle from the AMOS site from 2,000 cm<sup>-1</sup> to 5,000 cm<sup>-1</sup> (2-5  $\mu$ m). The transmittance shows strong absorption by atmospheric  $H_2O$  and  $CO_2$ . The OH(v) spectra was obtained by running a line-by-line code [13] assuming OH(v,j) populations created at 8 km s<sup>-1</sup>. The  $H_2O^*$  spectra was obtained by running a high temperature non-equilibrium code [14] at  $T_r = T_v = 1,500$  K. This is a best guess at the  $H_2O^*$  internal temperature. It is interesting that the OH(v) and  $H_2O^*$  spectral signals are somewhat separated in wavenumber. From this analysis, it is clear that the  $H_2O^*$  source radiance will be much more attenuated by the atmosphere than the OH(v) radiance. We, therefore, expect that most of the signal reaching AMOS will be from OH(v).

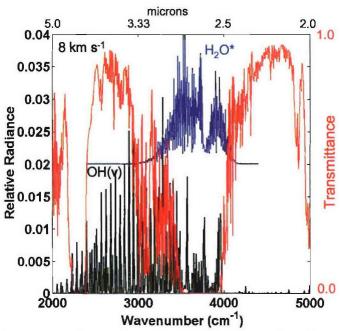


Figure 6. Normalized spectral radiance from OH(v) (black curve) and  $H_2O^*$  (blue curve) at 8 km s<sup>-1</sup> relative collision velocity. The OH(v) and  $H_2O^*$  curves have been separately normalized to 1.0 and the  $H_2O^*$  curve displaced for clarity. The atmospheric transmittance for a 60 degree zenith look angle from AMOS is shown in red. Spectral resolution is 5 cm<sup>-1</sup>.

Figure 7 shows the total (un-attenuated) source, summing both OH(v) and H<sub>2</sub>O\* contributions at 8 km s<sup>-1</sup>, as well as the total (attenuated) apparent signal. The apparent signal was obtained by multiplying the source signal by the atmospheric transmittance at each spectral bin. The integrated total apparent signal is decreased by a factor of 0.249 by the atmosphere according to this analysis. Because most of the atmospheric attenuation occurs in the same spectral region as the H<sub>2</sub>O\* contribution, a very large part of its contribution to the signal disappears in the apparent spectra.

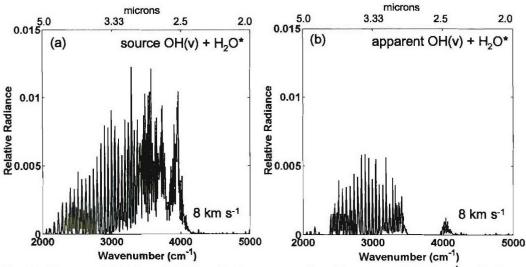
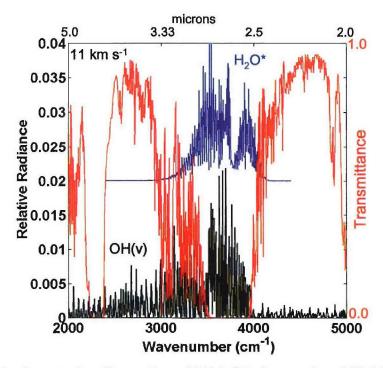


Figure 7. (a) Source  $OH(v) + H_2O^*$  relative spectral radiance at 8 km s<sup>-1</sup> relative collision velocity. (b) Apparent  $OH(v) + H_2O^*$  relative spectral radiance at 8 km s<sup>-1</sup> relative collision velocity. Here, the  $OH(v) + H_2O^*$  signal has been attenuated by the atmosphere.

Figure 8 shows OH(v) and  $H_2O^*$  source signal at 11 km s<sup>-1</sup>. The  $H_2O^*$  internal temperature is assumed to be the same as for the 8 km s<sup>-1</sup> case. The higher collision velocity, however, shifts the OH (v) spectra to higher energy so there is much more overlap with the  $H_2O^*$  contribution. This shift also puts the OH(v) contribution much more into the spectral region with large atmospheric attenuation.



**Figure 8.** Normalized spectral radiance from OH(v) (black curve) and  $H_2O^*$  (blue curve) at 11 km s<sup>-1</sup> relative collision velocity. The OH(v) and  $H_2O^*$  curves have been separately normalized to 1.0 and the  $H_2O^*$  curve displaced for clarity. The atmospheric transmittance for a 60 degree zenith look angle from AMOS is shown in red. Spectral resolution is 5 cm<sup>-1</sup>.

Figure 9 shows the total (un-attenuated) source summing both OH(v) and  $H_2O^*$  contributions at 11 km s<sup>-1</sup>, as well as the total (attenuated) apparent signal. The integrated total apparent signal is decreased by a factor of 0.187 by the atmosphere according to this analysis. It is interesting that, although we expect more source signal at higher relative velocities (ram firing), we also expect more atmospheric attenuation.

It is useful to report the total signal in Watts integrated spatially over the entire radiating region and spectrally across  $2-5 \mu m$  that would be observed from AMOS including atmospheric attenuation following the above analysis. We expect this estimate to be an upper bound on the observable radiation. We use the following equation, following Eq. 3, to perform the estimate,

Total Signal (Watts) = (Efficiency in photons per  $H_2O$  from Figure 5) (#  $H_2O$  from engine s<sup>-1</sup>) (3.33e3 cm<sup>-1</sup> / photon) (1.9863e-23 Joules / cm<sup>-1</sup>) (atmospheric attenuation factor). (5)

The results are given in Table 1 for 8 km s<sup>-1</sup> and 11 km s<sup>-1</sup>.

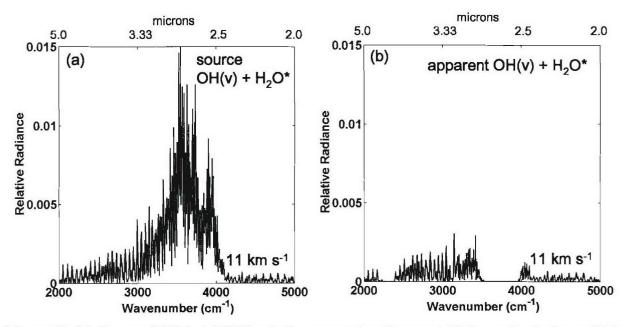


Figure 9. (a) Source  $OH(v) + H2O^*$  relative spectral radiance at 11 km s-1 relative collision velocity. (b) Apparent  $OH(v) + H2O^*$  relative spectral radiance at 11 km s-1 relative collision velocity. Here, the  $OH(v) + H2O^*$  has been attenuated by the atmosphere.

Table 1. Total Signal Estimates for Shuttle PRCS Engine Firings Including Atmospheric Attenuation in the 2-5  $\mu$ m pass-band. Efficiencies include contributions from OH 2.8  $\mu$ m, OH(v), and H<sub>2</sub>O\*, H<sub>2</sub>O 2.7  $\mu$ m, as shown in Figure 5.

Relative Velocity (km s <sup>-1</sup> )	Efficiency from Figure 5 (OH 2.8 μm+ H <sub>2</sub> O 2.7 μm)	PRCS Engine # H <sub>2</sub> O s <sup>-1</sup>	Atmospheric Attenuation	Total Signal (Watts)
8.0	0.0538	1.42e25	0.249	1.26e4
11.0	0.214	1.42e25	0.187	3.76e4

Previous observations from AMOS of two PRCS engine firings simultaneously at 11 km s<sup>-1</sup> report a signal of 6.3e4 Watts  $\pm$  50% in a somewhat narrower spectral region [6,8]. For a single engine, as assumed in the present analysis, this gives an approximate total signal of 3.15e4  $\pm$  50% Watts, which is well matched by the 3.76e4 Watts at 11 km s<sup>-1</sup> given in Table 1.

#### 6. INSTRUMENTATION

A total signal estimate from the Space Shuttle PRCS plume in the 2-5 μm band allows an assessment of available sensors and measurement feasibility. The basic measurement approach consists of integrating a spectrometer onto one of the large telescopes at the AMOS facility. The B37 1.2 m telescope has been identified as available for visiting experimenters [15]. This particular telescope has a 3 mrad total field-of-view (FOV) which would encompass only 2.3 km of plume assuming a 60° view angle from zenith. A telescope with at least 8 mrad FOV is really needed to collect most of the expected plume emission. The B37 telescope might still be acceptable since collecting a good spectrum is the priority, and as long as there is sufficient signal-to-noise (S/N). A good spectrum, in this case, would be a plume measurement at 4 cm<sup>-1</sup> spectral resolution. This would allow identification of key reactions and species. Though a

4 cm<sup>-1</sup> spectrum would be ideal, 8 or even 16 cm<sup>-1</sup> would still be useful. Two different spectrometer systems are currently under consideration. These are discussed in the proceeding paragraphs along with some initial S/N estimates.

The small size, ruggedness, and fast scanning capability of ABB's (formerly Bomem) 200 series Fourier Transform Infrared (FTIR) Spectroradiometer make it a potential candidate. A currently available system operates with two simultaneous detectors; an InSb covering 1-6 μm and an MCT covering 2-15 μm. Its basic specifications are listed in Table 2. Both detectors are liquid nitrogen cooled. The 1 cm<sup>-1</sup> Noise Equivalent Spectral Radiance (NESR) is 1.37e-09 and 1.4e-08 W/cm<sup>2</sup>-sr-cm<sup>-1</sup> for the InSb and MCT detectors respectively. Both values were measured with a 1 sec integration time. The NESR at other resolutions and integration times can be estimated from

$$NESR_{v} = \frac{NESR_{1}}{v\sqrt{t}}$$
 (6)

where  $NESR_1$  is the NESR at 1 cm<sup>-1</sup>,  $\nu$  is the wavenumber resolution, and t is the measurement time.

Resolution (cm <sup>-1</sup> )	1	2	4	8	16
Frame Rate (scans/sec)	10.3	18.6	31.4	47.8	64.6
Max Acquisition Time (sec)	95	104	125	163	242

Table 2. ABB 254 FTIR Spectrometer Specifications.

Assuming the spectrometer FOV is filled (via some telescope system), a radiance can be generated using the total signal estimate from the preceding section and by assuming plume emission from a spherical region of space. An average apparent radiance is given by

$$L^a = \frac{P}{4\pi A} \tag{7}$$

where  $L^a$  is the apparent radiance, P is the total power in Watts, and A is the plume area. To calculate an S/N, the NESR was converted to a Noise Equivalent Radiance (NER) by multiplying by the bandwidth (3000 cm<sup>-1</sup>). This assumes a constant NESR over the 2-5  $\mu$ m band which was found to be reasonable for this initial analysis. The S/N is then just given by

$$\frac{S}{N} = \frac{L^a}{NER} \,. \tag{8}$$

Figure 10 shows the calculated S/N for the InSb detector at the available spectral resolutions and up to 15 seconds of frame co-addition. A plume diameter of 5 km and a total signal of 3.76e04 W (11 km/s case) are assumed. The results are not encouraging as no S/N values were above 1. Further, the current configuration for the B37 telescope would not meet the spectrometer total FOV assumption. The spectrometer collimator has a 45 mrad FOV and a 6.4 mm entrance aperture.

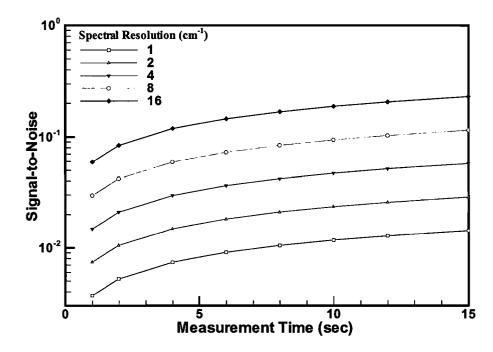


Figure 10. Estimated signal-to-noise for various spectrometer spectral resolutions and measurement times.

The emission analysis did not include any  $H_2O$  or OH overtone radiation below 2  $\mu m$  which could help improve the overall S/N. Also, the new 300 series spectrometer currently being offered by ABB has a factor of 2 improvement in sensitivity. However, according to the above results, at least one order of magnitude and probably two orders of magnitude improved sensitivity are needed for a good measurement.

Another possible sensor is the Broadband Array Spectrograph System (BASS) owned and operated by the Aerospace Corporation [16]. It is a dispersive type spectrometer with a 3-13.5 µm spectral range. This instrument has a stated noise equivalent power (NEP) of 4.0e-14 W/sqrt(Hz) for a 1 second integration time. The sensor would not capture any emission from OH or H<sub>2</sub>O below 3 µm but most of that may be absorbed anyway (see Figure 9b). Since this instrument disperses the energy into separate detectors, a per-pixel S/N estimate was obtained. Unfortunately, this required dividing the total signal estimate up into a spectrum. A rough estimate for the 3-4.2 µm (2400-3333 cm<sup>-1</sup>) region was accomplished by assuming approximately 60% of the total energy was emitted equally over this region (see Figure 9b). Utilizing the radiance calculation from equation 7 and the solid angle of the AMOS B37 telescope, a spectral irradiance was estimated with

$$E_{\lambda} = \frac{0.6L^{a}\Omega_{t}}{\Delta\lambda},\tag{9}$$

where  $\Omega$ , is the telescope solid angle and  $\Delta\lambda$  is 1.2  $\mu m$ . The S/N was then calculated from

$$\frac{S}{N} = \frac{E_{\lambda} A_{t} \Delta \lambda_{d} \sqrt{t}}{NEP}, \tag{10}$$

where  $A_t$  is the telescope primary mirror area,  $\Delta\lambda_d$  is the approximate pixel spectral resolution (0.1  $\mu$ m) in that wavelength region, and t is the detector integration time. Assuming a 1 sec integration time, an S/N of approximately 1448 was calculated. While this seems very encouraging, there would be a price. Near the 3  $\mu$ m spectral region, a 0.1  $\mu$ m difference between pixels translates to over 100 cm<sup>-1</sup> difference in wavenumber. The spectral resolution would be far lower than that desired. As with the FTIR spectrometer, the analysis also assumed that all the energy collected by the telescope was input into the BASS spectrometer. The results of these calculations for the BASS sensor were not reviewed and approved by any Aerospace Corp. personnel.

### 7. CONCLUSIONS AND FUTURE WORK

We have presented an estimate of the total signal level of radiation in the 2-5 µm region of Shuttle PRCS engine firings that could be observed from AMOS. The analysis is based on very recent work on the chemical mechanisms which give rise to the radiation, involving production of excited OH and H<sub>2</sub>O species formed from collisions of atmospheric O-atom and H<sub>2</sub>O from the engine exhaust. Our analysis includes effects of the attenuating atmosphere and an estimate of the spectral distribution of radiation. Our results for the total signal are in good agreement with a previous observation from AMOS of PRCS engine firings, giving us confidence in the overall analysis.

One weakness of the present analysis involves assumptions about how much collisionally excited H<sub>2</sub>O radiates in the 2-5 µm band. Future work will involve obtaining better estimates of the excited H<sub>2</sub>O contribution through use of quantum scattering techniques. It may also be possible to extract this information from simulations of the excited H<sub>2</sub>O spectra obtained from classical trajectory calculations [17]. Another important consideration in assessing the feasibility of ground-based observations is the spatial distribution of radiation. Modeling of the spatial distribution will require use of a reacting flow code and an analysis similar to that done in [3].

The initial analysis indicates that the ABB FTIR spectroradiometer would not have the sensitivity to measure the Space Shuttle plume emission under full FOV conditions. Perhaps, a large telescope with a short focal length (i.e., fast optics) could be one way to increase the signal into the ABB spectrometer. The BASS sensor, on the other hand, may have the sensitivity required, but at the cost of lower spectral resolution. Further investigation into various infrared spectrometers and telescope arrangements is clearly needed.

#### 8. REFERENCES

- 1. G.E. Caledonia, "Infrared Radiation Produced in Ambient/Spacecraft-Emitted Gas Interactions Under LEO Conditions," AIAA paper 00-0104 (2000).
- L.S. Bernstein, R.A. Dressler, Y. Chiu, J.O. Wise, J.A. Gardner, A.L. Broadfoot, M. Braunstein, P. Sydney, and E. Murad, "Temporal Dependence of the Spectral Content of LEO Spacecraft Engine-Exhaust Atmospheric Interactions," 2004 AMOS Conference, Maui, HI (2004).
- 3. W.L. Dimpfl, G.C. Light, and L.S. Bernstein, J. Spacecraft and Rockets, 42, 352 (2005).
- 4. D.K. Zhou, W.R. Pendleton, Jr. G.E. Bingham, D.C. Thompson, W.J. Raitt, and R.M. Nadile, J. Geo. Res. 99, 19,585 (1994).
- 5. R.E. Meyerott, G.R. Swenson, E.L. Schweitzer, and D.G. Koch, J. Geo. Res. 99, 17,559 (1994).
- 6. L.S. Bernstein, J.B. Elgin, C.P. Pike, D.J. Knecht, E.E. Murad, T.F. Zehnpfennig, G.E. Galicia, and A.T. Stair, Jr., J. Geo. Res. 101, 383 (1996).
- 7. D.P. Murtagh, E.J. Llewellyn, and P.J. Espy, Geo. Res. Lett, 24, 85 (1997).
- 8. D.L. A. Rall, I.L. Kofsky, C.P. Pike, D.J. Knecht, and T. P. Zehnpfennig, Journal of Spacecraft and Rockets, 33, 393 (1996).
- 9. L.S. Bernstein, Y. Chiu, J.A. Gardner, A.L. Broadfoot, M. Lester, M. Tsiouris, R. Dressler, and E. Murad, J. Phys. Chem. 107, 10695 (2003).
- 10. M. Braunstein, R. Panfili, R. Shroll, and L. Bernstein, J. Chem. Phys. 122, 184307 (2005).
- 11. G. Karabadzhak, Y. Plastinin, E. Szhenov, A. Afanasiev, and B. Khmelinin, "Preliminary Analysis of Exhaust Plume Radiation during Soyuz-TM Retro-firings," 34th AIAA Thermophysics Conference and Exhibit, AIAA Paper 2000-2373, Denver, CO, (2000).
- 12. P.K. Acharya, A. Berk, G.P. Anderson, N.F. Larsen, S.-Chee Tsay, and K.H. Stamnes, "MODTRAN4: Multiple Scattering and Bi-directional Reflectance Distribution (BRDF) Upgrades to MODTRAN," SPIE Proceedings, Optical Spectroscopic Techniques and Instrumentation and Space Research III, Volume 3756, (July 1999).
- 13. L.S. Rothman et al, "The HITRAN molecular spectroscopic database: edition of 2000 including updates through 2001," J. of Quantitative Spectroscopy and Radiative Transfer 82, pp. 5-44 (2003).
- R.L. Sundberg, J.W. Duff, and L.S. Bernstein, "Nonequilbrium infrared emission model for the wake flow of re-entry vehicles," J. of Spacecraft and Rockets, vol 30, pp. 731-741 (1993).
- 15. AMOS User's Manual, Det 15, Air Force Research Laboratory, Kihei, Maui, Hawaii, Rev 12, (April 2001).
- J.A., Hackwell D.W. Warren, M. Chatelain, Y. Dotan, P. Li, D. K. Lynch, D. Mabry, R.W. Russell, and R. Young, "A Low Resolution Array Spectrograph for the 2.9-13.5 μm Spectral Region," Proc. SPIE Conference 1235 on Instrumentation in Astronomy VII (1235), 171-180 (1990).
- 17. D.W., Noid M.L. Koszykowski and R. A. Marcus, "A spectral analysis method of obtaining molecular spectra from classical trajectories," J. Chem. Phys., 67, 404 (1977)